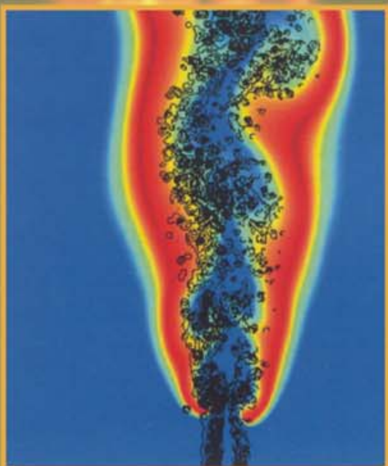
Improving Industrial Burner Design with Computational Fluid Dynamics Tools:

Progress, Needs, and R&D Priorities



Workshop Report

September 2002

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About this Workshop Report

Burner designers, burner end-users, combustion researchers, and computer code developers participated in a workshop on September 6 and 7, 2001, to explore the role of computational fluid dynamics (CFD) tools in the design of industrial burners. The workshop centered around three questions: 1) What has CFD done well? 2) What has CFD not done well? and 3) What CFD improvements are needed? Burner designers shared their experience using CFD codes with other burner designers and CFD modelers. CFD modelers shared the current state-of-the-art in the modeling and simulation of combustion and fluid mechanics phenomena that is relevant to the burner design process. After the presentations, experts participated in a facilitated discussion. Burner designers identified the successful uses and limitations of current CFD methodologies and models. Experts from the burner design and modeling communities then collectively identified the priority research needed to enhance burner design. Recognition and appreciation is extended to the workshop participants who contributed their time and expertise to developing the start of a research plan. The workshop agenda and a list of participants are provided in the appendix to this report.

The U.S. Department of Energy's Office of Industrial Technologies (OIT) and the Sandia National Laboratories (SNL) sponsored the workshop. The workshop was held at the Sandia Combustion Research Facility in Livermore, California. Robert Gemmer led the effort at OIT, and Dr. Robert Gallagher led the effort at SNL. The workshop was facilitated by Melissa Eichner and Diane McBee of Energetics, Incorporated. The workshop report was prepared by Melissa Eichner.

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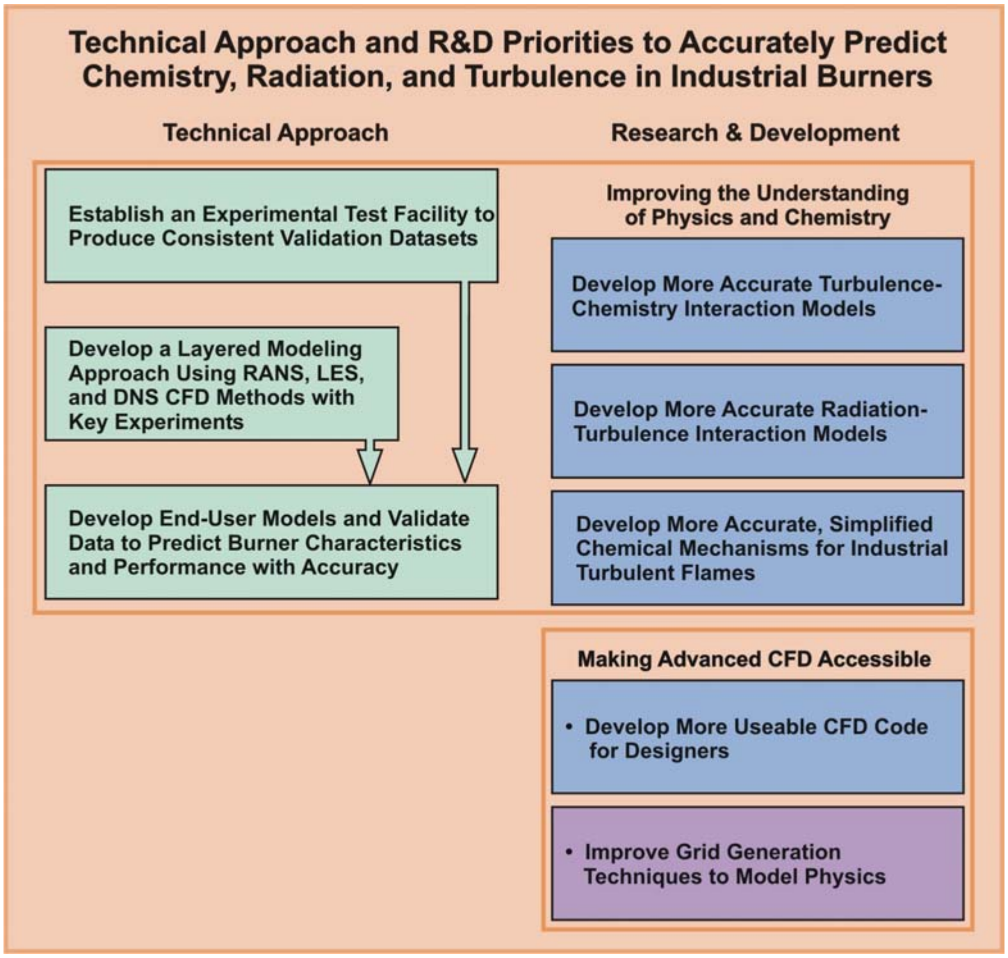
I. Executive Summary

Industry relies on heat from burners in all combustion systems. Optimizing burner performance is critical to complying with (progressively more) stringent emissions requirements and to improving industrial productivity. Even small improvements in burner energy efficiency and performance can have significant impacts in a continuous operation, more so if the improvements can be used in other combustion systems and across industries. While tremendous advances have been made in understanding the fundamental science of combustion, the remaining challenges are extremely complex. Today, trial and error is the only satisfactory burner design and problem-solving approach. To make improvements, it is critical to understand and accurately predict how heat is released and transferred to a load. Computational fluid dynamics (CFD) offers a numerical modeling methodology that helps in this understanding. Existing CFD tools are not fast, accurate, or cost-effective enough and, hence, are not used to their potential today.

A coherent near-term and long-term CFD development strategy is needed to understand and control the intricately coupled burner phenomena of chemistry, turbulence, and radiation in models, as well as the chemical kinetics. The elements of this strategy are presented in Exhibit E1. A sustained investment by a broad coalition of stakeholders will realize the improvements in performance, energy savings, and environmental management in industry, transportation, and defense.

Advanced CFD technology will be incorporated into progressively more robust tools over time that can be used to improve the design of new and retrofitted equipment as well as in operational problem solving. The benefits to industry and society will come through enhanced energy efficiency from more efficient transfer of heat to the load; reduced NO_x, SO_x, CO, and particulate emissions; use of alternative energies; improved product quality; reduced development costs; better burner designs; and faster problem diagnosis with expanded response options. By 2010, the industrial energy savings could be nearly 100 TBtu and $50 million in operating expenses per year. By 2020, the savings from this technology could be on the order of 1 quad and $1 billion per year, based on assumptions of a 1% market growth and up to 8% efficiency savings in new combustion equipment. The operating expense reductions will come mostly through emission control savings, with burner development and technical service cost savings also contributing.

Exhibit E1. Priorities to Improve Industrial Burners



Delivering Heat with Burners in an Industrial Process—A Primer

Burners are an integral part of boilers, furnaces, and process heaters. To supply heat for an industrial application, fuel is burned in a burner in the presence of an oxidant (either air or oxygen). The fuel type used depends on the application, combustion equipment, and fuel availability. Fuels used include natural gas, petroleum, byproducts, coal, wood, and biomass. Each fuel has unique heat values, byproducts, and emissions formed when burning; flammability (concentration at which the fuel burns); and other factors that impact overall performance.

In combustion systems, the goal is to transfer the heat from the burning fuel to the *load*. The heat emitted by the burner is transmitted through materials (boiler walls, tubes) and space (air) and absorbed by the load—water in the case of boilers; metals and chemicals in the case of furnaces/process heaters. If the heat is transferred more efficiently, less fuel and energy is wasted.

Combustion is initiated with a spark, and the burn is often fueled continuously in industrial operations. Maintaining the optimal ratio of fuel and oxidant is essential to burning the fuel completely (using all its heat value) and regulating the temperature. For example, unburned fuel increases emissions and possible contamination, while non-optimal temperatures contribute to NO_X formation. Burners are difficult to operate optimally because of the complex physics and chemistry involved, turbulent mixing as the heat radiates, how the heat will be used, shapes and size of the container, as well as many other factors. Because of the lack of understanding about what takes place in the combustion systems, tradeoffs often have to be made between optimizing performance and reducing emissions. Industrial combustion operations today are typically designed and managed by trial and error.

Burner users want to be able to predict how to heat the load efficiently while achieving rigid emissions reductions. The combustion challenges of end-users are diverse, often requiring customized solutions. Burner design tools are used to optimize fuel and air mixing, energy release, and heat delivery for a specific process or load. Numerical models are a set of design tools used to predict burner characteristics and performance in order to meet end-user requirements. Even small improvements can have significant impacts in a continuous burning operation, especially if the improvements can be used in other combustion systems and across industries. Quantitative CFD design methods will improve energy efficiency; reduce NO_x, SO_x, CO, and particulate emissions; facilitate alternative energy use; improve product quality; reduce development costs; enable better burner designs; and allow faster problem diagnosis with expanded response options. Consequently, R&D investments to improve burner performance could have a significant impact on the economy and the environment.

II. CFD R&D Priorities for Improved Burner Design

1. Introduction

Industry relies on heat from burning fuel in a burner. Even small improvements in burner efficiency can have significant economic and environmental impacts.

Regulatory and competitive forces are pushing combustion equipment manufacturers to improve performance, lower environmental impact, enhance control, and increase fuel flexibility. While tremendous advances have been made in understanding the fundamental science of combustion, the remaining challenges are extremely complex. Improving burners—an integral part of all combustion systems—to comply with progressively more stringent emissions requirements and to improve industrial productivity will require a focused research and development effort and significant breakthroughs. Combustion currently accounts for over 75 percent of industrial energy use. Even small improvements in performance can have large impacts on a continuously operating process, and if these improvements were realized across combustion equipment, the energy savings and emissions reductions impact could be enormous.

Trial and error is the only satisfactory burner design approach used today. Understanding and controlling the intricately coupled burner phenomena is essential to the design of next-generation burners.

Optimizing burner performance to meet end-user requirements is a complex process that typically requires consideration of the entire integrated turbulent combustion system. The coupled effects imposed by turbulence-chemistry interactions, radiation heat transfer, and detailed chemical kinetics must be controlled in complex wall-bounded flows so that optimal performance and minimal emissions are achieved. To make improvements, it is critical to understand how heat is released and transferred to a load. CFD are numerical modeling codes that help in this understanding. Exhibit 1 offers an outline of some of the variables involved in optimizing burner performance.

There is currently no satisfactory burner design approach other than trial and error, and there is a fundamental lack of validated predictive models and complimentary experimental data. Understanding and controlling the intricately coupled phenomena encountered in typical industrial configurations is extremely important for the design of next generation burners.

Exhibit 1. Examples of Burner Optimization Considerations		
Fuel and Air Mixing	**Combustion (Energy Release)**	**Delivery of Heat to a Specific Process or Load**
• Fuel type (gas, liquid) • Temperature control • Injector configuration (shape, angles) • Enclosure geometry	• Chemical kinetics: - Ignition - Sustainability - Stabilization - Emissions • Enclosure geometry • By-product optimization • Environmental issues: - Waste heat - Pollutants (NO_x, CO_2, other) - Soot (carbon)	• Flame shape • Flame velocity • Optimizing heat to load: - Radiant heat transfer - Convection heat transfer • Process specific geometries

2. Enhancing Burner Design with CFD: Progress to Date

Today's CFD tools do not accurately predict burner performance—which is required to meet emissions reductions and other end-user requirements—but they contribute to burner design and diagnosing problems.

CFD tools are currently used to improve burner performance in two distinct areas: in the design cycle and in trouble-shooting to solve problems that occur during operation. Exhibit 2 describes how CFD is used to enhance burners.

Exhibit 2. CFD Tools: Two Applications with Burners

Burner Design Process – Developing a burner for a specific application requires the 6 steps outlined below. CFD tools are used in each step (except prototype fabrication) to develop the prototype burner and evaluate it in simulated environments and for optimizing fabrication. CFD is used to help designers achieve end-user requirements. The accuracy of the CFD design tool determines how fast the steps can be completed and the confidence with which the designers are able to apply the results from testing. More advanced CFD tools will reduce the development time and the number of iterations, both are needed to meet rigorous end-user requirements and commercial success.

1. Define the requirements for mixing, combustion, and delivery in a specific application
2. Design prototype with design codes and prediction analysis
3. Fabricate prototype
4. Assess performance and characterize
5. Evaluate the prototype in simulated and real environments
6. Develop and optimize a fabrication process

Burner Trouble Shooting Process – CFD tools are used to troubleshoot flow, mixing, combustion, and heat transfer problems in every type of combustion system—from dryers to boilers to glass melting furnaces. More advanced CFD tools would permit more rapid and robust solutions of customer problems.

CFD tool development has progressed steadily over the last two decades. CFD tools have contributed to improved designs and the solution of a vast array of burner- and combustion-related problems in propulsion and power systems, including rocket motors, gas turbine engines, reciprocating engines, furnaces, and heat exchangers. CFD has provided qualitative insight leading to improved engineering accuracy, operation, and increased product output and emissions control. Among the notable successes are helping to increase the efficiency of combustion turbines and reducing emissions of NO_x, unburned CO, hydrocarbons, soot, and char from engines and furnaces. Exhibit 3 lists further contributions of CFD to burner design.

Exhibit 3: Contributions of CFD to Burner Design

- Predicting catastrophic failure
- Qualitative trends and parametric analysis
- Visualization for customers
- Non-reacting gaseous flows (treatment of gaseous phases is more accurate than liquid and solid phases)*
- Quantitative analysis of gas velocity and temperature patterns
- Qualitative analysis of radiation heat transfer*
- Flame dynamics and shape
- Flame interaction
- Effects of simple geometries
- Models of temperature and heat release patterns and qualitative trends associated with major species*
- Integration of detailed burner code with heating process

* Further improvement in CFD capabilities could significantly enhance burner performance in these areas.

However, while the contribution of these tools today is significant, they are unable to solve design problems in complex systems. The existing CFD models are largely empirical (i.e., providing qualitative insight based on trial and error), and the uncertainty associated with this empiricism significantly limits their applicability. End-user requirements for efficiency and emissions reductions will not be cost-effectively met with conventional empirical design.

There are also many uncertainties in the models used today. Model predictions with today's tools are often not in satisfactory agreement with experimental measurements, sometimes differing by several orders of magnitude. A model may predict well under a specific set of conditions, yet, if the conditions deviate, the model is incorrect. Predictions of priority combustion system performance characteristics, such as radiative heat transfer and pollutant emissions, are notoriously difficult or unreliable. Consequently, burner designers cannot accurately predict how to effectively reduce emissions with CFD. For example, today's tools cannot accurately predict mixing and fuel reactions.

Today's models for combustion and radiation are relatively simple as a result of past computational limitations and the long-standing requirement of fast turnaround times for calculations. Modeling approaches (e.g., to obtain accurate closure schemes for combustion) include the assumptions of fast chemistry, laminar flamelets, conditional moment closure (CMC), and probability density function (PDF) transport. Limitations associated with these approaches are presented in Exhibit 4. Trade-offs exist between model accuracy and the validity of the baseline modeling assumptions. For example, the combustion regime in contemporary combustion devices at atmospheric pressures is typically intermediate between flamelet combustion and distributed combustion. At elevated pressures, the flamelet approximation is rarely valid and distributed combustion modes become the norm.

Exhibit 4. Limitations of Current Modeling Approaches

- **Fast Chemistry:** The assumption of fast chemistry, while computationally simple and inexpensive, circumvents the estimation of the chemical source terms. Under this assumption the thermodynamic state is completely determined as a function of mixture fraction. Effects like ignition and extinction cannot be accounted for, and the formation of pollutants, whose rates of formation are kinetically limited, are poorly predicted.

- **Laminar Flamelets:** Laminar flamelet models assume that flame structures are thin in comparison to turbulent eddies. The laminar flamelet regime is considered to be an ensemble of strained laminar flames that only depend on mixture fraction and scalar dissipation. While computationally efficient, there is considerable debate on the applicability of this method to flames outside of this regime, especially at elevated pressures.

- **Conditional Moment Closure (CMC):** The CMC method solves transport equations of conditionally averaged quantities instead of the spatially filtered counterparts. Variables upon which the chemical reactions are known to depend must be identified and are chosen as conditioning variables. While CMC tends to be more global, solving transport equations in conditioned space adds further dimensions to the problem. With these dimensions come additional modeling issues, approximations, and the related uncertainties.

- **Probability Density Function (PDF) Transport**: PDF transport methods solve a transport equation for the filtered joint PDF of species, energy, etc., to represent *sgs* interactions within a statistical hyper-volume. The filtered chemical source terms occur in closed form within the transport equation of the joint-PDF. The dimensionality, however, increases with the number of species, and unclosed molecular mixing terms must be modeled. In addition to the uncertainties associated with the molecular mixing terms, PDF transport methods do not take time-history effects into account.

Burner designers are reluctant to use existing models because they are difficult to use and the quality/reliability of the results depends too strongly on the training and experience of the user (i.e., how codes are used). Given the time, money, and skill required for applying them to new problems, CFD tools are not used to their potential today. Overall, the tools are not fast enough, accurate enough, or cost-effective enough to use in a wide range of applications.

End-users want better, more affordable burners. The development of a more quantitative and validated CFD capability can help end-users meet their greatest challenge—accurately predicting NO_X formation and radiative heat transfer.

The goal of end users is to have better, more affordable burners and combustion systems, as outlined in Exhibit 5. They want burner designs that are responsive to application requirements and properly integrated into the entire combustion system. Replacing empirical testing with computer simulations will offer marked savings in development costs. New, higher performing burners will be developed in less time, and will be better able to do the job they are intended to do. Problems will be diagnosed quicker and with increased reaction options.

The performance and efficiency of industrial burners can be significantly improved with the development of a more quantitative, validated, and accurate CFD capability. New CFD tools will more accurately and quantitatively incorporate the underlying physics, chemistry, and fluid dynamics, (e.g., pressure, flow, and flame characteristics) needed to minimize or eliminate the empirical approach to combustion system design and address end-user requirements, including fuel flexibility, system efficiency, profitability, and NO_x, CO, and particulate emissions. Burners can be developed that work properly over a full range of specifications and conditions, while improving overall performance, decreasing emissions, and increasing equipment life. Improved tools will make it easier for non-specialists to model burner performance and consistently deliver more accurate results.

The R&D priorities needed to encourage the incorporation of existing scientific understanding into the code as well as to improve the predictive capability of models that are precursors to code development are discussed in the following section.

Exhibit 5. Goal and Objectives of End-users

GOAL: Better, more affordable burners

Objectives:
- Design burners that are responsive to end-user requirements, especially:
  - Accurately predict NO_X formation, particulate matter, and other emissions
  - Accurately predict radiation heat transfer
  - Improve controls and turndown ratio
- Integrate burners with plant overall balance
- Replace burner tests with simulations
- Prioritize burner improvements based on the value to burner users (e.g., return on investment)

Improved CFD will ensure faster development of burners that are better able to do the job they are intended to do. To meet industry's needs, burner designers and operators must be able to accurately predict NO_x formation and radiation heat transfer.

3. Technical Approach and R&D Priorities to Accurately Predict Chemistry, Radiation, and Turbulence in Burners

Understanding and integrating the coupling of mathematical descriptions of chemistry, turbulence, and radiation into models as well as the chemical kinetics are significant, complex challenges. Breakthroughs in these areas will transform industrial combustion systems—and the economy.

A coherent near-term and long-term CFD development strategy is needed to address the complex challenges facing designers of industrial combustion systems. Exhibit 6 presents this strategy, which focuses on accurately predicting chemistry, radiation, and turbulence in industrial burners. The strategy will develop the needed technical approaches, improve the understanding of physics and chemistry, and make advanced CFD accessible to commercial code developers. These priorities, discussed in this section are based on an analysis of workshop results presented in Appendix A (Results Developed Sequentially at the Workshop).

To significantly enhance burner performance in the near term and long term, the R&D priorities focus on improving fundamental understanding. Systematic analysis is required based on a carefully blended combination of experiments, experimental diagnostics, and numerical simulations. The experiments will provide general qualitative and quantitative insights and detailed validation data. The validated simulations will provide additional quantitative information that is not directly obtainable experimentally with a high degree of confidence. The ongoing development of bigger, faster computers and compatible software will contribute significantly to an improved modeling capability.

Technical Approach—Developing CFD Design Tools for Burners

Improving the predictability of burner performance with CFD design tools requires a technical approach involving testing, validation, and complex modeling based on an improved understanding of physics and chemistry.

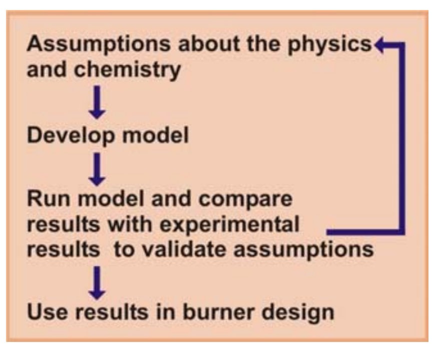
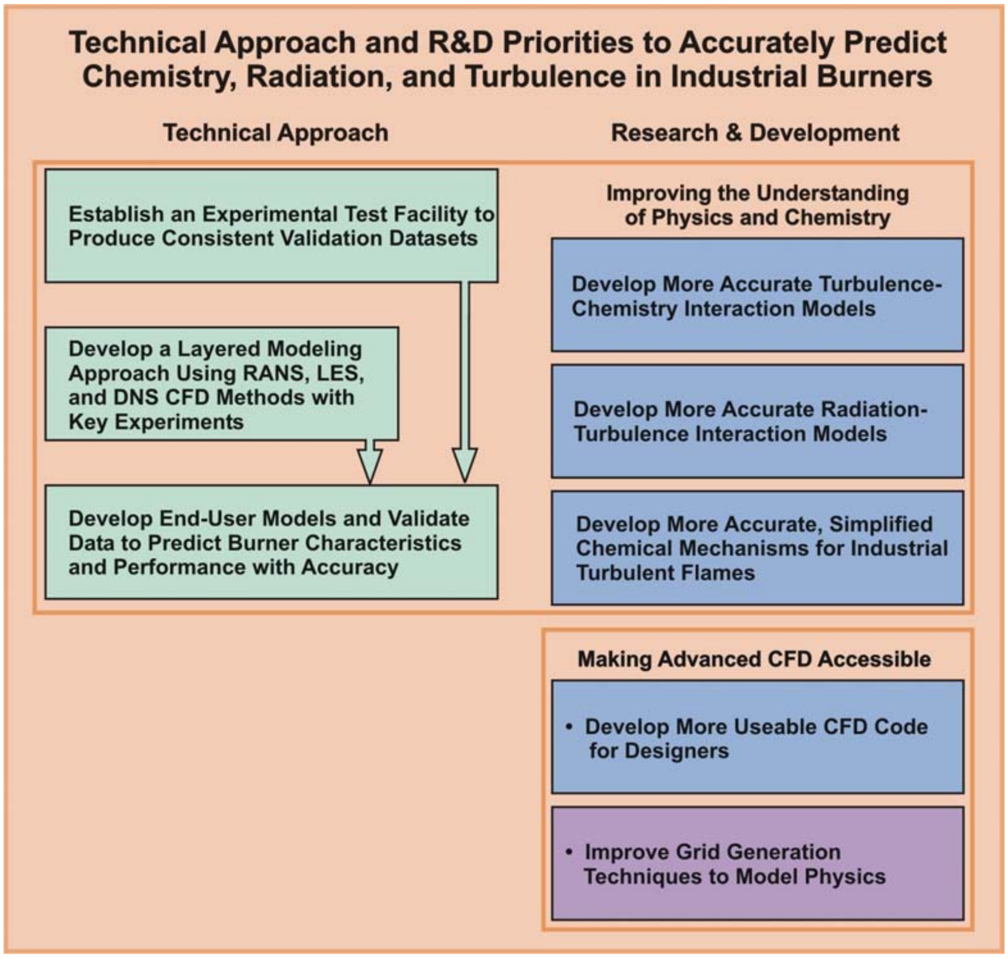


Exhibit 6.



<u>Establish an Experimental Test Facility to Produce Consistent Validation Datasets.</u>

Industrial code developers and designers need to be able to verify that the models accurately predict the chemistry and physics in an actual industrial process. Because it is too costly and risky to interrupt an industrial operation, researchers need a place where they can conduct experimental burner tests to determine the impact of impact of design modifications. An experimental facility is essential to developing a better understanding of physics and chemistry of industrial burners and predictive modeling capability. The failure of models to accurately predict in-use systems cannot be explained without consistently collected data. These smaller scale experiments need to be conducted in well-defined and controlled conditions. All phenomena should be monitored with precise diagnostic techniques (e.g., interactions of velocity, temperature, heat flux, and major species). Experimental results should be compared with model predictions to determine the accuracy of the model. The validated datasets will be used to validate other models, again comparing measurements to calculated values. Validated datasets collected on a consistent basis will become a resource that can assist other designers.

Priority: **<u>Develop a Layered Modeling Approach Using RANS, LES, and DNS CFD Methods with Key Experiments</u>**

Using models of different scales and scope simultaneously (i.e., layered) is an effective strategy to interlink complex data that can then be used in more comprehensive models. The widely used Reynolds-Averaged Navier-Stokes (RANS) approximation, Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS) are existing CFD approaches used in modeling burner phenomena that could be improved and layered. The strengths and tradeoffs of these models are presented in Appendix 2. Systematically interlinking these three models can tap the strengths of each.

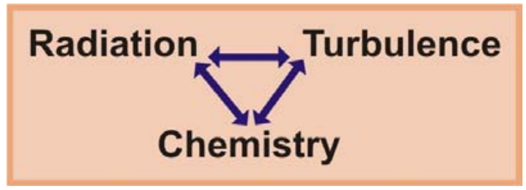
Conducting fundamental validation experiments is a central part of developing the layering process. For example, experimental data can be linked with the results of numerical analysis for a common set of operating conditions. With this approach, models can be developed that more accurately represent fluctuations over space and time among turbulence, chemistry, and physics for a given combustion system. Interactions and tradeoffs with different configurations, burners, and conditions can be better understood and used to optimize data requirements, reduce model complexity, and increase the speed and ease of computation. The layered approach can increase turnaround times and accuracy, overcome CFD limitations that exist today, and consider many variables simultaneously. The computational and scientific challenges such as modeling the extra artifacts/terms that result from simultaneously using equations must be addressed.

Priority: **<u>Develop End-User Models and Validate Data to Predict Burner Characteristics and Performance with Accuracy</u>**

End-users want to optimize burner characteristics and performance for a given load while meeting regulatory requirements. Predicting NO_X emissions and radiation heat transfer are typical priorities. Industrial models are used to predict variables in systems with various boundary conditions on both the bench scale and industrial scale. By developing consistent validation datasets through experimental testing and applying this understanding to a layered modeling approach, more accurate modeling schemes can also be developed. The complex models can be simplified for end-use while maintaining the accuracy of predictions.

Research & Development — Improving the Understanding of Physics and Chemistry

The complex interactions between radiation, turbulence, and chemistry must be better understood to develop advanced CFD tools and improve burner design. Major breakthroughs in these areas will enable industry to meet the emissions and performance requirements of end-users.



Priority: **Develop More Accurate Turbulence-Chemistry Interaction Models**

The mixing of reactants (fuel and air) within the burner creates motion that affects the chemistry and products of the reactions. As the gas expands, for example, it changes the turbulence within the burner. Because the interaction of fuel and air is not well understood, today's models are unable to accurately and reliably predict turbulence or chemistry. Appropriate treatment of chemistry is typically not included in modeling because of the limited understanding of fundamentals and the high computational costs. Consequently, there is uncertainty and error in the predictions, and the interaction effects are largely not addressed. Without accurate predictions of turbulence and chemistry, models are therefore severely limited. For example, if a chemical species is predicted incorrectly, the absorption coefficients for the radiative transport equation will be incorrect, even if the radiation model is correct. Innovative basic R&D breakthroughs are needed to revolutionize combustion system performance.

Priority: **Develop More Accurate Radiation-Turbulence Interaction Models**

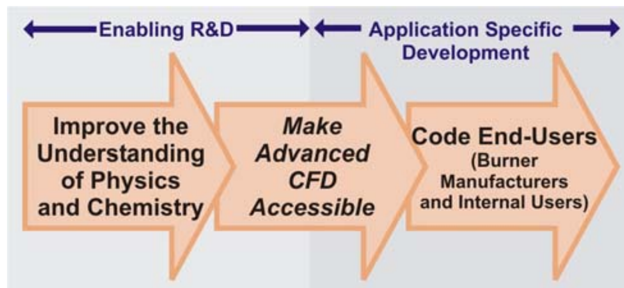
The goal in a combustion system is to transfer heat to the load. The radiation of heat (e.g., how energy is emitted, transmitted, and absorbed) is impacted by the chemical properties of the gas, particulates and other materials within a combustion enclosure, as well as material density. Today, the physics of the radiation heat transfer process is understood but the material radiation properties are not, while the cost of computation in terms of run times is too high. As a result, the material radiation properties and their interaction with turbulent motion cannot be predicted with accuracy and absorption and scattering efficiencies used in models are incorrect. Predicting NO_X and other parameters reliably depends on the development of an accurate radiative heat transfer model.

Priority: **Develop More Accurate, Simplified Chemical Mechanisms for Industrial Turbulent Flames**

Predicting burner characteristics and performance requires an understanding of all the interactions taking place throughout the entire combustion system. For example, the complex chemistry and physics of three-dimensional flames must be understood in detail to develop predictive capabilities. Once developed, this understanding must be simplified to a manageable number of equations/sub-models for use by end-users. This approach needs to be applied to complex fuels including solids and liquids. The detailed mechanisms and the reduced mechanisms that are good representations must be experimentally tested. Systematically developing these chemistry mechanisms, along with consistent validation data, will yield a resource that can be used throughout the burner design community. It is an essential part of to the technical approach to model development.

Research & Development—Making Advanced CFD Accessible

Once the fundamental understanding of physics and chemistry is integrated successfully into advanced validated models, R&D is needed to make the advanced CFD more accessible to non-experts. Pre-competitive advancements to assist with CFD code development and the integration of fundamentals into gridding methods will accelerate the commercial application into burner design.



Priority:

Develop More Accurate and Useable CFD Codes for Designers

End-users want CFD tools that are affordable, easy to use, and include the fundamentals. Today, industry is often 10 years behind in terms of the scientific modeling of physics, chemistry, and modeling. While the market will determine when and how advanced CFD gets integrated into industrial design tools, embedding the results of radiation, chemistry, and physics research into engineering-level CFD code requires additional R&D by the scientific/research community. For example, researchers need to develop scaled-down models addressing a specific class of industrial problems to reduce the level of expertise required to apply CFD. This R&D will assist CFD code developers to use the improved data and modeling capability with confidence, and will help the advanced code find its way into the commercial market. Integrating the advancements into CFD code as they become available will assist end-users meet progressively more stringent requirements.

Priority:

Improve Grid Generation Techniques to Model Physics

Better techniques are needed to generate grids for routine use of CFDs. Also, grid independent solutions are difficult to achieve. Mathematical challenges exist for generating both modeling grids and CFD to assist with data reduction and predictability.

4. Benefits and Impacts of Developing Modeling Methods and Data to Simulate and Accurately Predict Chemistry, Radiation, and Turbulence in Industrial Burners

Quantitative CFD tools can be applied to the design of all burners used in both new and retrofit equipment throughout the world. In addition, the tools are used in trouble shooting and problem solving throughout industry. The breakthroughs in fundamental understanding of chemistry, turbulence, and radiation interaction as well as chemical kinetics can also benefit transportation, defense, and other applications.

The benefits and impacts of these tools on burner characteristics and performance are significant, as described in Exhibit 7. As an enabling tool, it is difficult to estimate the potential impact of the R&D on industry and society. The improvements will be incorporated in progressively more robust design tools over time. By 2010, industrial energy consumption could be reduced by nearly 100 TBtu and $50 million in operating expenses per year. By 2020, the savings could be on the order of 1 quad and $1 billion per year. These savings were calculated assuming a 1% market growth and up to 8% efficiency savings in new combustion equipment by 2020 as presented in Appendix D. The operating expense reductions are mostly in emission control savings, although burner development and technical service cost savings also contributed. Further analysis needs to be conducted to substantiate these savings.

Exhibit 7. Benefits and Impacts of Quantitative CFD Design Methods

- **Improved Energy Efficiency**—heat is transferred to the load more efficiently, thereby reducing fuel use
- **Reduced NO_x, SO_x, CO, and Particulate Emissions**—emissions characteristics can be predicted to achieve desired emissions profiles, thereby reducing pollution and the costs associated with regulatory compliance and non-compliance
- **Facilitates Alternative Energy Use**—combustion system impacts from alternative fuels can be evaluated, thereby contributing to energy security
- **Improved Product Quality**—byproducts that contact the load can be reduced and temperature can be more reliably controlled, thereby producing more consistent products
- **Reduced Development Costs**—relying on simulations to evaluate design options reduces fabrication and testing time and costs, and reduces the reliance on trial and error
- **Better Burner Designs**—optimally designed burners that are integrated into the entire combustion system are more responsive to application requirements
- **Faster Problem Diagnosis with Expanded Response Options**—more rapid and robust solutions to customer problems improves performance and reduces manpower requirements and downtime

5. Conclusions and Next Steps

A sustained investment in a coherent near-term and long-term CFD development strategy is needed to address the complex challenges facing designers of combustion systems. Benefits in terms of improved performance and energy savings will accrue to industry, transportation, defense, and environmental management. All stakeholders, industry- and government-wide, should collaborate to leverage the needed resources.

The priorities presented in Section 3 represent a coherent strategy to make a significant impact on burner performance in the short term and the long term. The technical approach and R&D priorities provide the building blocks to meet end-user requirements. These priorities can be used by industry, DOE, and other funding agencies to guide the development of research plans for burner design improvement. Preliminary next step actions to address the priorities for improving the understanding of physics and chemistry are presented in Exhibit 7 at the end of this section.

Key technical conclusions and noted strategies to get started are as follows:

- **More robust CFD tools can be used to help industry improve burner performance and meet regulatory requirements (e.g., NO_X), both in the short term and, to a greater extent, in the long term.** Knowledge exists today that can be integrated into various codes and used immediately. Advancements in fundamental chemistry, turbulence, and other key physics could make a significant impact in the next 3 to 7 years.

- **Turbulence-chemistry and radiation-chemistry interaction modeling must be a core focus for burner improvement.** Future research should focus on developing scientific- and technology-based CFD for burner design models rather than an empirically based.

- **A coordinated validation effort is needed that focuses on key industrial problems is needed.** Benchmark data sets are needed for model validation and to perform accurate model comparisons. A coordinated beta testing and benchmarking program is needed involving users, commercial model developers, experimentalists, and researchers. The validation effort must foster communication between experimentalists and modelers to ensure the development of application-relevant experiments that use hardware and impose minimal uncertainties associated with boundary and flow conditions.
    - Highly resolved data sets need to be developed, maintained, and made publicly available to evaluate a range of models.
    - Funded projects are needed that promote interaction between experimental and numerical researchers, code developers, and burner end-users that have code preferences.
    - End-users need to identify what the models should do and over what range of conditions. Models focus at different levels and the costs vary accordingly.

Researchers need to educate end-users about the limitations of individual models.

- **The outstanding modeling challenges of industrial burner combustion are the same as those of gas turbines and clean coal combustion devices. The combustion end-user and research community will need to join together and speak as one voice in order to secure the necessary R&D funding.** Government-wide collaboration could help share the costs and focus the scientific mind trust of the country on improving performance and energy efficiency across many end-use applications. An immediate area for collaboration is understanding and modeling turbulence-chemistry interaction, which has many applications, including industry, transportation, defense, and environmental management. Strategies will need to be developed to meet the criteria for project selection, which vary by government agency.

- **End-users need to maintain a dialog with researchers and commercial vendors so that needed improvements are integrated in respective codes. They also need to foster the transfer of understanding from universities and National Laboratories.** End-users would like to see the existing understanding integrated into code as soon as possible. Workshop strategies that provide an opportunity for experimentalists and modelers to work together need to be developed and fostered. The modeling community must specify the important problems requiring collaboration. This will ensure that fundamental models are correctly implemented.

Exhibit II.7: Initial Approach and R&D Next Steps for Improving the Understanding of Physics and Chemistry

Technical Approach

Develop an Experimental Test Facility to Produce Consistent Validation Datasets

- Identify synergies and collaborations between models
- Identify key experiments for applications

Develop a Layered Modeling Approach Using RANS, LES, and DNS CFD Methods with Key Experiments

- Identify industrial needs
- Conduct experiments that validate useful and practical code, and cover a range of complexity and difficulty
- Synergize/coordinate results with fundamental validations
- Develop exothermic chemical energy recovery, especially to avoid refrigeration
- Enhance polymer stabilization, especially to withstand heat exposure during transportation and storage
- Develop radically new polymerization
- Prevent degradation during processing

Research & Development

Improving the Understanding of Physics and Chemistry

Develop More Accurate Turbulence-Chemistry Interaction Models

Develop More Accurate Radiation-Turbulence Interaction Models

- Develop cross-discipline discussion across government funding programs
- Assess model shortcomings and define industry's needs
- Use workshop results to develop request for proposal (RFP)
- Propose project to close the gap between need and shortcomings
- Develop good validation data for the model
- Develop benchmarks to identify needed inputs for success
- Characterize radiation transfer properties

The next-step actions are nearly the same for these two priorities. There are important differences between the two but not at the level of detail specified in this exhibit

Develop More Accurate, Simplified Chemical Mechanisms for Industrial Turbulent Flames

- Apply an expanded "GRI-like" approach to more complex fuels, including solids and liquids
- Measure unique value of "GRI-like" R&D and communicate value to funding agencies
- Develop methods to automatically reduce mechanisms linked to detailed mechanism
- Develop good flame data

Appendix A. Workshop Agenda and Participants

Exploring the Role of Computational Fluid Dynamics Tools for Industrial Burner Design

Sandia Combustion Research Facility, Livermore, CA
September 5 – 7, 2001

AGENDA	
TIME	**ACTIVITY**
Wednesday, September 5, 2001	
6:30 pm	Reception
Thursday, September 6, 2001	
7:00 am	Badging and Registration
7:00 am	BREAKFAST
8:00 am	***Welcome***
8:15 am	***Presentations from Burner Designers*** Woody Fiveland, Alstom Power, Inc. Mike Henneke, John Zink Co. Jon Berkoe, Bechtel Corp.
10:30 am	BREAK
10:45 am	**Facilitated Discussion 1: *Challenges with Burner Design***
12:30 pm	LUNCH
1:30 pm	***Presentations from CFD Modelers*** Eddy Chui, CANMET Energy Technology Center Joe Oefelein Sandia National Laboratories
3:00 pm	BREAK
3:15 pm	***Facilitated Discussion 2:*** **CFD Modeling R&D Needs to Enhance Burner Design**
5:00 pm	Adjourn
6:30 pm	DINNER
Friday, September 7, 2001	
7:00 am	BREAKFAST
8:00 am	***Facilitated Break Out Session:*** **Implementation Actions and R&D Next Steps**
10:15 am	BREAK
10:30 am	**Consensus on Recommendations**
12:00 pm	Adjourn
12:00 pm	LUNCH

CFD Burner Workshop Participant List
September 6 & 7, 2001

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Appendix B: Modeling Burner Phenomena: Tradeoffs, Algorithmic Requirements, and Validation Requirements

Tradeoffs in Simulating and Modeling Burner Phenomena

The three fundamental choices for simulating and modeling the burner phenomena are the widely used Reynolds-Averaged Navier-Stokes (RANS) approximation, Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS). They each provide a unique contribution.

Reynolds-Averaged Navier-Stokes (RANS) approximation is the least numerically intensive. For this approach all turbulent motions are modeled. The closure is empirical and based on scaling arguments that apply only in the time-averaged limit. In general, RANS predictions only give qualitative insight, are highly sensitive to models and model constants, and respective constants must be adjusted and tuned for every flow.

Large Eddy Simulation (LES) is a much more mathematically rigorous and numerically intensive methodology compared to RANS but offers a higher degree of accuracy in return. For this approach, the large energetic scales are resolved and the subgrid-scales are modeled to provide a complete time-accurate spatial representation of the full range of relevant scales. This is in contrast to the bulk representation provided by RANS. Thus, in contrast to RANS, LES closures are time-accurate, the models tend to be more universal, and it is not necessary to adjust constants for every flow. With the appropriate grid constraints in place, the use of dynamic modeling (described below) or more advanced simulation based models eliminates the need for any model constants.

Direct Numerical Simulation (DNS) is the most numerically intensive. For this approach all scales are resolved and no modeling is required. The primary limitation of DNS is that it is severely CPU limited. Performing a full-scale DNS is not feasible at this time. Because of this limitation, DNS can only be used for analysis of the smallest local scales associated with a given flow in simple periodic domains. Thus, LES represents the only viable alternative. The LES technique provides a framework that handles discrete multiple-time multiple-length scale closures in a mathematically rigorous manner. The requirements associated with LES, however, impose an extremely strict set of both algorithmic and modeling requirements.

Algorithmic Requirements of LES

Unlike RANS, the use of LES as a tool to provide a complete time-accurate spatial representation of the full range of relevant scales imposes an extremely strict set of algorithmic requirements that must be rigorously enforced. Numerical dissipation and dispersion errors can have significantly devastating effects on *sgs* models. The presence of these errors depletes energetic turbulence scales at the mid- to high-wavenumbers and consequently competes with the models. When this occurs, the *sgs* models themselves have little or no effect on the flow and the contamination often leads to erroneous conclusions. To avoid this situation, numerical methods used for LES must provide spatially “non-dissipative” spectrally clean damping characteristics out to the smallest wavenumbers coupled with simultaneous local conservation of mass, momentum and total-energy. An additional constraint is that the energetic scales need to be resolved on grids that minimize commutation errors.

No existing commercial CFD code-bases currently have spectrally clean algorithmic frameworks appropriate for LES (nor do many of the current LES research codes in the community). Because of the initial emphasis on RANS based methods (which are much less sensitive to dissipation and dispersion errors) the foundational algorithms used in most of the current solvers employ highly dissipative and dispersive techniques. These techniques are typically required to provide numerical stability. It is important to note that it is not trivial to convert such code-bases to LES since it involves much more than the implementation of a model. It is also important to note that the use and evaluation of state-of-the-art models in a dissipative numerical framework can lead to significant erroneous conclusions regarding the accuracy of the model and significance of the results.

Co-located schemes with explicit artificial dissipation terms added for stabilization purposes have historically failed to provide the appropriate spectral characteristics. This is easily shown if one compares the magnitude of the residual associated with the artificial dissipation terms of a given scheme to that associated with a given *sgs* model. The former is always orders of magnitude greater, even for higher-order schemes. Unfortunately, this fact precludes a wide class of flow solvers, including the trivial conversion of most RANS based codes. Fully conservative, fully implicit, or alternatively, semi-implicit staggered grid algorithms, on the other hand, have been shown to give acceptable spectral characteristics. The use of such schemes for LES and *sgs* model development represents a minimal requirement.

Validation Requirements of LES

Unlike the RANS approach, which averages over both the temporal and spatial scales, LES maintains both the temporal and spatial characteristics of the turbulence. Relevant dynamic processes include growth mechanisms (such as baroclinic vorticity generation), decay mechanisms (such as the cascade to smaller scales), and advection mechanisms (such as vortex pairing and stretching). The assumption that LES accurately captures these dynamical processes must be validated with a wide range of simultaneous measurements that quantify both the temporal and spatial coherence of the flow. This includes cold flow characteristics, initial and boundary conditions, time-averaged and unsteady measurements of velocity and scalar mixing processes, measurements of flame structure (curvature, wrinkling, and surface area), surface dynamics, chemistry, and reaction rates. A complete description of unsteady strain, strain-rates, amplitude, frequency, and curvature is also required along with the local instantaneous strain field. Eventually datasets that characterize flame stability, acoustic interactions, ignition and extinction phenomena will be required.

Appendix C. Results Developed Sequentially at the Workshop

This section presents the results of discussion that evolved over the course of the workshop. Priority design needs were identified along with priority CFD research and development needs. They are presented in Sections A and B, respectively. However, the reader will notice a discrepancy between the presentation of priorities in this appendix and Chapters I and II. The results presented in Chapter II are a carefully formulated strategy based on the information presented in this appendix.

1. Priority Needs of Burner Designers

The priority needs, as shown in Exhibit C.1, are organized into five categories: Mechanics of CFD, Products of CFD, Ensuring Confidence in Results, Flow-Flame Modeling Issues, and Alternative Approaches. In general, the latter two categories can be addressed by longer-term research, while progress in other areas can be implemented immediately or in the short term. Flow-flame modeling issues represent the key phenomena which must be systematically treated to provide the end products for CFD. The needs in Exhibit C.1 are prioritized based on 1) impact on end-users and 2) impact on design. The need with the greatest *impact on end users* is the development and validation of state of the art models. The need with the greatest *impact on design* is the development of more user-friendly code.

The top priority needs for burner designers are shown below.

Top Priority Needs for Burner Design

- ► Validation of Models
- ► NO_X Modeling
- ► Radiation Heat Transfer
- ► More Specific and User-Friendly Code
- ► Improved Gridding Methods to Model Physics

For each priority need, the key burner design and modeling issues are discussed along with the following: CFD R&D priorities to address the burner need; available resources existing today that are applicable to the need; and other related burner needs from Exhibit C.1.

For the priority needs below, the R&D timeframes when useful results could be expected are near-term (0-3 years), mid-term (4-6 years), and long-term (>7 years). The R&D priorities, indicated by the ★ symbol, are ranked across all the CFD R&D needs for the five top priority needs of burner designers. The range of possible R&D solutions was defined

Exhibit C.1: Priority Needs of Burner Designers

Mechanics of CFD

- More specific and user-friendly code ●●○○○○○○○○○
- Improved gridding methods to model physics ●●○○○○○○○○
- Specialized combustion models ○○
- Intelligence in results that provide confidence levels (internal checks) ○○
- Specify stoichiometric ratio verse flows as input to models
- Error bars to indicate confidence

Priority
● = Impact on End Users
○ = Impact on Design

Products of CFD

- NOx modeling ●●●●●●●●● ●●●○○○○○○○○
- Radiation Heat Transfer ●●●●●●●●●○○○○○
- Trace byproducts modeling (some algorithms are incorrect and too time consuming)
- Specific subset of multi-physics needed for NOx modeling:
  - Trace species
  - Heat transfer
  - Reacting flow prediction
  - Accurate mechanism with defined physics
  - Sensitivity to condition changes (turbulence, chemistry, radiation)
  - Complex chemistry understood
  - Lifted flame prediction improvement
  - Near burner field predictive capability

Ensuring Confidence in Results

- Validation of models●●●●●● ●●●●●●○○○○○○○○
- Benchmark problems to compare computing speed ●●●
- Validate systems with complex boundary ○
- Validate boundary conditions ○
- Need data base of properties and materials ●
- Need measurement data to prove success and validate total system and subsystems (in-process fields data, end data, isolated sub elements, generic property data, data specific to system, algorithms (solution reflects model) ○
- Reliable prediction of flow and heat transfer fundamentals

Flow-Flame Modeling Issues

- Unstable combustion ●●●○○○
- Accurate chemistry and compressible-flow modeling together ●●●●○
- Combined nozzle-mix and pre-mix combustion models ●○○○○
- Spray modeling ●○○
- Reliable flame surface modeling●●
- Improve LES turbulence modeling (substantial improvement over other models) ●○
- Flame-surface interaction (hot and cold surfaces) ●
- Pre-mix flame modeling ●
- Mixing within furnace ●
- Coupling convection section with CFD for overall furnace efficiency
- High-swirling flow modeling accuracy improvement
- Low-swirl burner modeling capability

Alternative Approaches

- Determine if a grid-based system is best – is there a new way?
- Multi-physics/coupling needs to be complete

broadly in terms of time horizon, level of effort, expenditure, and other factors. R&D needs fall into one of three categories:

1) Incremental improvement on existing commercial codes;
2) New code based on existing knowledge incorporating lessons learned, including from other fields; and
3) Research on new technology and approaches (e.g., non grid-based methods).

Detailed Discussion of Burner Design Needs

***Burner Design Priority Need*: Validation of Models**

The CFD R&D priorities to improve the modeling validation capability are presented in Exhibit C.2. The highest priority R&D need is to develop an experimental test facility to produce consistent validation data and make this data publicly available. Another priority is to collect data from real in-use industrial facilities. Key burner design and modeling issues related to model validation are outlined below.

- Burner designers need to be able to verify that respective codes reproduce the actual physics and chemistry. Although validation is often under-funded and under-emphasized, validation is essential to the development of accurate model and code bases. Models are sometimes validated experimentally in the laboratory yet fail in in-use systems with complex boundaries. This failure is a result of the poor quality of the input. With the absence of data, causes of failure cannot be explained.

- Accurate algorithms are needed so that the numerical solution reflects the model. Validation data that isolates the specifics of the models is needed. Modelers need generic property data, system-specific data, and validation data of subsystem and total system performance. They need to know temperature, flow, and species distribution inside the combustion chamber.

- A facility like the (currently un-funded) Burner Engineering Research Laboratory (BERL) is needed to collect data on a consistent basis for validation, along with protocols for data collection. By collecting data on a consistent basis, researchers can return to the facility and build confidence by testing the impact of design modifications, and any variability will be consistent. For example, gridding issues can be explored with confidence given one common geometry. Such a facility needs to be publicly available so everyone can use it and have access to the data. Vendors could use it to develop numerical and experimental data comparisons needed to validate code for users. While some facilities currently exist at universities and national laboratories to validate data on various types of systems, they do not provide the scope and specificity provided by BERL.

- Today's validation data has been collected in different ways on different systems and therefore cannot be compared. BERL provided detailed measurements of velocity, temperature, heat flux, major species, and OH, for example. This data was invaluable to validating code developed at the time. An enhanced validation facility that allowed testing across more conditions, different stochiometries, different burners and injector configurations is needed to validate the code. Facilities of different scales could be useful, but the scale of BERL is good for many purposes. An inventory of capabilities at all facilities is needed.

Exhibit C.2: Validation of Models

●●●●●●●●●●●●○○○○○○○○

Related User Needs:

- Benchmark problems to compare computing speed ●●●
- Validate systems with complex boundary ○
- Need data base of properties and materials to validate boundary conditions ● ○
- Need measurement data to prove success and validate total system and subsystems (in-process fields data, end data, isolated sub elements, generic property data, system-specific data, validation data, algorithms so the solution reflects the model) ○
- Reliable prediction of flow and heat transfer fundamentals

<u>Priority</u>
● = Impact on End Users
○=Impact on Design

Available Resources:

- Horizontal and vertical simulator is available
- Efforts are underway using a layered approach (not useful to all but a good first step)

CFD R&D Priorities:

<u>**Near-Term**</u>

- Develop one facility to produce consistent validation data and make data publicly available (consider reinstating BERL) ★★★★★★★★★★★
- Collect data from in-use industrial facilities – its difficult to get data due to logistics and cost ★★★★★★★★★
- Reduce manpower need to validate data (e.g., software tools) ★
- Translate R&D progress and activities to industry (need common terms) ★
- Include comprehensive data to validate CFD code (with licenses) ★

<u>**Mid-Term**</u>

- Use database to compare models
- Develop a series of models to validate commercial models (DNS) ★★
- Determine if data from an average boiler would be sufficient to validate model and provide enough boundary conditions

★ = R&D Priority

- Translating fundamental advancements at National Laboratories to the burner community has been difficult. An environment for direct interaction between lab personnel and industrial users is needed to provide a framework to enhance transfer of knowledge in applications. Generation of fundamental, burner-relevant datasets could be useful in building and validating sub-models. In addition, establishing a common nomenclature would help Lab experts translate the meaning and impact of advancements to an application, as well as help experts understand the needs of designers and end-users and how their insight can help. Scientific nomenclature used by fundamental researchers is often not used by industrial designers who use Btu per foot in lieu of scientific units.

- Data collected on laboratory or pilot scale or in-use systems are valuable, but several challenges currently exist: data is difficult to collect; not enough is known about the boundary conditions; operations are optimized for production (i.e., one condition) and not data collection; and, increasingly, utility unit operators are reluctant to allow data collection for proprietary reasons. Within a BERL-like facility, experiments can be designed so boundary conditions and other aspects are known with a high degree of confidence. One of the challenges of validation is designing with confidence an experiment that is modelable. To do this, the experiment must be built so that the boundary conditions are known and quantified, which is generally not how burner systems are built today. A critical threshold of data needs to be collected to be useful, and this requires a focused effort and considerable expense. Datasets that are relevant to advanced models including turbulence and turbulence interaction models are available. Comparing model predictions with experiments however, is time consuming. New software tools may be able to speed up design and reduce manpower time.

Burner Design Priority Need: **NO$_X$ Modeling**

The CFD R&D priorities to improve NO$_X$ modeling are presented in Exhibit C.3. Improved modeling of turbulence-chemistry interactions is the highest priority R&D need. Using a systematic layered model approach that optimizes the use of RANS, LES, and DNS is also a high priority research need. A layered approach would utilize the strengths of different types of CFD and incorporate the results from fundamental laboratory experiments. Combining CFD and empirical models would allow uncertainties in predicting temperature and other species and would not require going all the way to fundamentals to predict NO$_X$. Another priority R&D need is investigating chemical reduction schemes. Key burner design and modeling issues related to NO$_X$ modeling are outlined below.

- Burner designers would like to accurately predict NO$_X$. The scale of accuracy needed within the system varies among users. In existing NO$_X$ models, the underling physics in the model itself is not well defined and is out-of-date. The percentage of NO$_X$ reduction for a given configuration is not provided, but it is needed for design standards and would be valuable to end-users. Today, NO$_X$ can be predicted relatively accurately on the macroscopic scale from inlet to outlet.

- NO$_X$ is sensitive to atypical conditions in the combustor such as turbulence, turbulence-scalar mixing, turbulence-chemistry interaction, radiation heat transfer, chemistry, changes in stochimetry, radiative loading, and boundary conditions at the fundamental

Exhibit C.3: NOx Modeling

●●●●●●●●●●●●○○○○○○○○

Related User Needs:

- Trace byproducts modeling (some algorithms are incorrect and too time consuming)
- Specific subset of multi-physics needed for NOx modeling:
  - Trace species
  - Heat transfer
  - Reacting flow prediction
  - Accurate mechanism with defined physics
  - Sensitivity to condition changes (turbulence, chemistry, radiation)
  - Complex chemistry understood
  - Lifted flame prediction improvement
  - Near burner field predictive capability

Priority
● = Impact on End Users
○ = Impact on Design

Available Resources:

- Look at gross output verses small scale
- Empirical methods are already good–flow, temperature, and heat distribution; UAW; and major species need improvement
- GRI Mechanism is more understood and can add to CFD codes
- Combine CFD with empirical methods to allow some uncertainty (good-enough chemistry)

CFD R&D Priorities:

Near-Term

- Use a layered approach that uses RANS, LES, and DNS[1] ★★★★★★★★★★★
- Develop improved chemical reduction schemes ★★★★★★★★★★
- Develop alternative algorithms for coupling chemistry with fluid dynamics★★★★
- New empirical NOx models tailored to specific conditions★★★
- Share empirical methods – technology transfer
- Integrate out details to simplify and track only a few species

Mid-Term

- Develop CFD for other uses: direct use for design; generating data bases for design code; validation
- Collaboration using CFD could produce good NOx results quickly (put chemistry in the model)
- Develop improved turbulence chemistry interaction models★★★★★★★★★★★ ★★★★★
- Predict chemistries ★★★★★★
- Use computational chemistry to predict NOx and improve NOx modeling (quantum chemistry) (radiation heat transfer)★
- Develop implementable, broad models that are available to everyone and share data/results ★

★ = R&D Priority

[1] High fidelity models and simulations to mediate between experiments and user code

chemistry level. Consequently, characterization and prediction over the entire range is needed, not just averages. Accordingly, the code will need to carry complex information. Accurate prediction of heat transfer along with chemistry is needed to successfully model NO_X. Most parameters may need to be predicted accurately to have accurate NO_X rediction.

- Currently, NO_X is typically not predicted from code but rather from empirical correlations. Improvements to the underlying combustion models will improve the overall design capability from empirical results—including improving the understanding of NO_X. This includes reliably predicting combustion flow and heat transfer properties of the system, which is challenging to get for design standards. Needed improvements to the underlying combustion model include improving the prediction of flow distribution, velocity, pressure, temperature, heat flux distribution, major species (e.g., CH_4, CO, CO_2, N_2, O_2), and intermediate species (e.g., OH, acetylene). Predicting flame lift off and near-burner flow-field is especially important for NO_X prediction. While improving the underlying combustion model will improve NO_X prediction from empirical data, it is unclear how this will impact prediction of NO_X from code.

- The understanding of the chemistry of NO_X formation has advanced in recent years. However, GRI-Mech is currently out-of-date and more accurate information has been obtained since GRI-Mech development ceased. Improvements would involve incorporation of more accurate species thermodynamic chemistry and reaction rates.

- Compiling implementable quantitative models of different areas of chemistry could benefit the community if it was made publicly available and used with confidence, especially above C1 and C2.

- The long-term strategy for reduction of NO_X in various applications will be the development of alternative approaches because upgrading existing approaches will not solve the challenges. Development of alternative approaches is costly and would have a much larger customer base than the burner community. A broader stakeholder group with common interests could be organized to address these issues and achieve the level of investment needed. The stakeholders include both government and private organizations, including DOD, NASA, DOE, national laboratories, and universities. Software, infrastructure, and advanced knowledge that can contribute to the effort exist today or are under development in various government offices.

- Another approach for improved NO_X is using a GRI-Mech-like approach ahead of time, then performing CFD simulations using only a few species. This would provide the possibility of treating detailed complex chemistry but only solving a few species equations. Manifolds are a great technique but are currently time-consuming to develop.

- Two approaches were offered to improve NO_X immediately or in the next year: 1) research shows that the flow-through ratio controls NO_X with pre-mixed flames, regardless of size, with the exception of sheared and quenched flames (e.g., flames for 15 kW to 1 MW lie on a narrow band); 2) existing CFD capabilities to predict NO_X can be used with higher order Reynolds stress and turbulence models and user-defined functions, including better chemistry in the model. This approach, using existing CFD code, would lead to good predictions that can be used as a baseline, although it will not be accurate.

***Burner Design Priority Need*:** **Radiation Heat Transfer**

The CFD R&D priorities to improve radiation heat transfer are presented in Exhibit C.4. Understanding radiation and turbulence interaction is the highest priority R&D need, followed by the application of a band-to-band approach. Key burner design and modeling issues related to radiation heat transfer are outlined below.

- Radiation heat transfer limitations are a prime source of errors in temperature predictions, with the degree of error varying from system to system. Users today are relying on gray solutions. Non-gray solutions that consider angular space so surfaces are not skewed are needed to predict heat flux.

- Speed of calculations is a major limitation in most radiative calculations, especially for shadow effects where P1 methods are not helpful. Alternative strategies can be developed to speed up calculations, and models with different degrees of complexity can be useful. For example, starting simple and staging the complexity of discrete ordinates as the answer gets closer is an option (e.g., starting with a S2 approximation and building to S4 and then to S6 later in the calculation so a full blown discrete ordinates (DO) solution is not necessary early on—P1 could be used early on to get a rough solution). Technology exists to do progressive stages of complexity, This approach needs to be implemented in the code.

Exhibit C.4: Radiation Heat Transfer

●●●●●●●●●○○○○○

Related User Needs:

- Soot modeling

Priority
● = Impact on End Users
○ = Impact on Design

Available Resources:

- Determine how to use alternate strategies of computing–use stages of increasing complexity for discrete ordinances (e.g., Monte Carlo)

CFD R&D Priorities:

Near-Term

- Add the interaction between radiation and turbulence to models (LES models) ★★★★★★★★★★★★
- Needs to be solved in a band-to-band approach (need correct models)* ★★★★★★★★★
- CK distribution methods may be useful to specify properties*

Mid-Term

- Grid clustering: separate grids for radiation and CFD*

Long-Term

- Multiple grids on geographically distributed processors*

★= R&D Priority
* Related to Mechanics of CFD

- Monte Carlo is the best method but is time consuming; it is expected to become more prominent as computers get faster. One possibility to speed up calculations is using a separate grid for radiation verses the flow. Radiation is concerned with temperature and species concentration gradients. This approach could reduce the number of grid points needed compared to a greater number needed for flow. The downside is that this would require communication between two grids. Multiple grids on geographically distributed processors will speed computing in the next five years.

- The current understanding of the interaction between radiation and turbulence flows is not available in today's models but could be added. Approaches from other fields should be considered.

- The radiant heat transfer calculation methods are well developed and the physics behind them well known. These methods are not commonly used in current code but could be added. The complexity of gridding greatly impacts the robustness of discrete ordinate radiation. With tetrahedral and unstructured grids, it is more difficult to devise efficient calculations, and it is expensive compared to rectangular grids. To improve numerical efficiency, researchers could focus on the wave front rather than the entire stream. Currently, the model distreetizes the equation to the different ordinantes, and each ordinate has a convection diffusion equation. The next step is to solve the convection diffusion equation like other equations.

Burner Design Priority Need: More Specific and User-Friendly Code

The CFD R&D priorities to make code more specific and user-friendly are presented in Exhibit C.5. Key burner design and modeling issues related to simplified and user-friendly code are outlined below.

- Front-end interfaces for burner design do not currently exist, although they could be adapted from other industries. The use of CFD codes requires users to have expertise in computers, CAD, graphic visualization, as well as fluid dynamics. A user-friendly GUI written with non-expert users in mind that guides the user through the process step-by-
-

Exhibit C.5: More Specific and User-Friendly Code

○○○○○○○○○

Related User Needs:	Available Resources:	CFD R&D Priorities:
		Near-Term
Specialized combustion models ○○	CFX has mix tank templates as an example	Develop front end that does not require an expert to use
Intelligence in results that provide confidence levels (internal checks) ○○	Web based applications, easier applications	Develop templates
Specify stoichiometric ratio verse flows as input to models	Use visual basic to streamline/develop front end	Scaled down versions that only include specific variables
Error bars to indicate confidence		

Priority
● = Impact on End Users
○ = Impact on Design

step is needed to decrease the start-up costs. In addition, users would like scaled down versions or templates for a specific class of problems to limit the amount of user input or switches. For example, boiler geometries are similar (hopper, burner holes, nose) with varying dimensions. The main templates could be scaled and could complete the GUI automatically. Other industries may already do this.

- A trend toward web-based systems in the future could help take the burden off users and avoid the need of dedicated specialized staff. Internet-based systems could run on clusters with users only paying when they use the code. Expert systems could guide users regarding where to adapt and control the solution process with smart solvers.

- Users want models that are simple to use and more affordable yet include the fundamentals. Research is needed to link CFD models, especially simplified (lumped) models.

Burner Design Priority Need: Improved Grid Generation to Model Physics

The CFD R&D priorities to improve gridding are presented in Exhibit C.6. Automatic generation of hybrid unstructured meshing using hexahedral is by far the highest priority R&D need. Key burner design and modeling issues related to gridding are outlined below:

- Improved gridding methods are needed to better represent the physics so models will be more accurate. Today, grid generation often takes longer than the run. Gridding methods cannot manage radiant heat transfer and flame spread, which are important to burner design. Over-reliance on tetrahedral gridding and the poor quality of tetrahedral meshing limit modeling capability. It is also difficult to get a grid independent solution. The source of the problem is not modeling theory but the size of grids available.

Exhibit C.6: Improved Gridding Methods to Model Physics

●●○○○○○○○○○

Related User Needs:

- Improve mesh quality for tetrahedral grids (mesh smoothing) ○○○○

● = Impact on End-Users
○ = Impact on Design

Available Resources:

- CAPRI may help speed with geometry exports
- Research is underway to increase speed (tetrahedral, etc. and entire CFD community)

CFD R&D Priorities:

Near-Term

- Structured grid methods with cut-cell geometry representation★★
- Unstructured grid generation improvement (R&D in progress)
- Release lab advancements on meshing incrementally
- Assess what is the best way to grid a model (update periodically)
- Identify resolution requirements
- Consider a change to solver verses meshing techniques ★
- Develop more flexible gridding for commercial code (autogen of structured grids)

Long-Term

- Automatic generation of hybrid unstructured meshing using hexahedral ★★★★★★★★★
- Alternative meshing strategies (AMR)

★ = R&D Priority

- Meshing takes too long. For unstructured grid generation, if time-dependent calculations are needed and adaptive gridding is used (i.e., matching the grid to the solution), then grid generation is part of the calculation. This is too time-consuming and expensive. Subdivision algorithms are also time-consuming.

- Streamlining the development of an initial grid is needed. Today, a solid geometry is created, followed by a grid, which is time consuming and buggy. When moving from solid models to gridding, geometry export is a problem because the geometries have different meanings for different CAD codes. A CAD-independent interface (e.g., CAPRI) can be used for geometry export and gridding the solid model up. Currently, direct CAD connectivity is being used to avoid the clean-up process entirely. While automatic meshing is used as far as possible. It can be done with tetrahedral; however, the issue with tetrahedral is not meshing but rather edge proximity (closed edges on automatic surface meshing), which increases accuracy of the solver before the automatic hexahedral meshing "go-carts" (i.e., Cartesian subdivisions) are used. With this method, code is written from scratch starting with a domain and divided up into fine regions and orthogonal mesh optimization or rounded edges.

- At the labs, methods have been developed based on Cartesian meshing and cut-cell representations of geometries with local refinement for efficiency. This combination is

- being developed for non-industrial applications and this is attractive from a grid generation standpoint because a workstation can compute a collection of surface triangulations (not just wedded surface) to a grid in minutes. Developing grid methods with cut-cell geometries will require substantial retooling and effort to address solver problems and disperzation methods.

- An emerging area is hexahedral grids which have received significant support from NASA. While challenges still exist, the approach offers promise.

- Tetrahedral grid generation is mature. Surface meshing on enclosed volumes and algorithms are used to mesh it up, and research is being conducted to allow automatic meshing of surfaces. Once done, tetrahedral meshing is close to automatic, while hexahedral meshing is difficult to solve. The use of tetrahedral meshing is avoided because of degradation of numerical accuracy. The primary research thrust for burners is the development of automatic generation of hybrid meshes using hexahedral as much as possible.

- Minimizing exposure to tetrahedral meshes is done because of accuracy issues, not because of degradation of cell convergence, memory, or solver performance.

- To develop better geometries to solve complex physics of heat transfer needed for burner applications, an automatic block scheme of structured grid would be better than refining an unstructured method. Most CFD code has abandoned the multi-block structured grid approach, instead moving to an unstructured approach that would be a major undertaking to reverse. However, the decision regarding hexahedral verses tetrahedral is the more important question (not unstructured versus structured). Every structured grid can be represented as unstructured. A structured grid can only be hexahedral. Block grid or multi-block grid can run with an unstructured solver. Concern exists over the ability to follow the wave front and know proximity relationships. An optimized Cartesian structured solver is being used with both a structured and unstructured mesh.

- Further research is needed to develop a robust, fast unstructured grid generation. Research is underway at the National Laboratories to help realize this opportunity. The National Laboratories have research underway on unstructured grids, a Cartesian structured adaptive approach, various hybrid grid generation methods that limit the number of tetrahedral cells as much as possible, and the development of efficient linear and non-linear solvers for both structured and unstructured systems. Vendors and National Laboratory researchers should identify how incremental advancements can be utilized.

- Users would like to have prudent recommended practices for selecting the best way to get the best grid for a combustion simulation, both today and in the future as knowledge advances.

- Packages exist today to mesh any geometry with tetrahedral cells, but this produces inaccurate results. One approach might be to change the solver so the meshing techniques do not have to change, though this is controversial. If we use new tetrahedral grids that are smoother and have a better quality and accept that the solvers are not going to get as accurate and reliable results as hexahedral, tradeoffs could maybe be made based on run-time requirements. For example, more run time for hexahedral is needed to get equivalent accuracy. For industrial process applications with limited access to computer power, the trade offs between tetrahedral and hexahedral need to be weighed. Which is the best meshing strategy for industrial applications? What quality of the solution is needed for industrial combustion, diffusion issues, and flame shape? Hybrid options are available that allow tetrahedral meshing in the internal volume and use hexahedral meshing to patch to the boundary. Is this a good approach? A Cartesian grid provides a more robust and accurate solution. Achieving the same degree of accuracy with a tetrahedral grid would require significantly more mesh resolution, which may be difficult to run in a production mode unless access to expensive computer systems exist.

- The burner-CFD community needs to identify resolution requirements and constraints with different types of grids. Users would like to have commercial code implemented with more flexible and productive gridding options, including blocking for structured grids in regions where this can be done (i.e., automatic generation of structured grids that break down without hybrid regions and without introducing non-orthogonality).

2. Priority CFD R&D to Address Burner Design Needs

By increasing the use of CFD in burner design, more effective and better performing systems will be made available to the industrial community. Five CFD R&D priorities have been identified that will provide the building blocks to address burner design needs in a broad range of industrial applications. This strategy emphasizes scientific and technology based methods that can be applied to various applications, geometries, and conditions rather then emphasizing an empirical approach. The latter approach does not change with variable conditions that are typical in industrial processing. With some exceptions, today's burner CFD is largely empirically based, yet more advanced CFD capabilities do exist and others can be developed.

Top Five CFD R&D Priorities

- ► More Accurate Turbulence-Chemistry Interactions
- ► More Accurate Radiation-Turbulence Interactions
- ► More Accurate Approaches to Simplified Chemistry for Industrial Turbulent Flame
- ► Develop a Layered Approach Using RANS, LES, DNS, and Key Experiments
- ► Develop an Experimental Test Facility to Produce Consistent Validation Datasets

The capability of CFD models today is limited by computer power. As computers get faster, the turnaround time and accuracy will improve. The research plan for CFD needs to consider what can be achieved in the next year and over the next decade. Existing tools can be used to accelerate the development of RANS and other models with experiments that can lead to results in the near term and help to refine the models in the future.

The five priorities are discussed below in more detail.

Detailed Discussion of CFD R&D Priorities

CFD R&D Priority: <u>Understand Turbulence-Chemistry Interaction and Develop Accurate Models</u>

- Today's models are unable to accurately and reliably predict turbulence or chemistry. For example, they do not reliably replicate what fuel does in a combustor. Current mixing models are inadequate, and appropriate treatment of chemistry is typically not included because of the limited understanding of fundamentals and high computational costs. Consequently, there is uncertainty and error in the predictions. Effects are also strongly coupled. If the chemical species found in the system are predicted incorrectly, the absorption coefficients for the radiative transport equation will be wrong, even if the radiation model is correct.

- Turbulence-chemistry interaction modeling is an issue with many applications, across industry, transportation, defense, and environmental management. Internal coordination across government funding agencies is needed to share the costs and realize the benefits for all stakeholders. Basic R&D is required. Broad, open-minded researchers will need to propose ideas and demonstrate that they work.

CFD R&D Priority: Understand Radiation-Turbulence Interaction and Develop Accurate Models

- Radiation issues in combustion are focused on heat transfer as well as photon interaction with chemistry (quantum chemistry). Material radiation properties cannot be predicted with accuracy, especially with gas and particles. Consequently, absorption and scattering efficiencies are incorrect. An accurate radiative heat transfer model is needed for reliable NO_X prediction.

- One near-term approach to model the interaction of radiation and turbulence is to run radiation with LES and use time averaging with RANS.

CFD R&D Priority: Develop Accurate Chemical Reduction Schemes for Industrial Turbulent Flames

- Reduced kinetic mechanisms are needed to couple the chemistry with CFD. To apply complex chemistry to three-dimensional flames, researchers need to have good mechanisms and be able to reduce it to a manageable number of species (e.g., 20). The development of detailed mechanisms should be linked to reduced mechanisms that are good representations so they can be tested. To do the chemistry, a coherent approach to developing mechanisms is needed so it is only done once. Detailed mechanisms will need to be developed in conjunction with a testing facility to produce consistent validation data such as BERL.

- End-users need to substantiate the value of mechanisms and communicate the need to potential funding agencies (e.g., determining the number of customers using full mechanisms for industrial use today and surveying the number of papers published using mechanisms or reduced versions). The GRI-Mech mechanism was developed for natural gas. This approach needs to be reinitiated and expanded to include more complex fuels, including solids and liquids.

CFD R&D Priority: Develop a Layered Model Approach For Validation Using RANS, LES, and DNS with Experimental Results

- A systematic approach to interlinking models can tap the strengths of different types of CFD and tie to fundamental experimentation. In the absence of empirical data, models can be used to validate other models. Used together, the RANS, LES, and DNS trio is a possible strategy. LES mediates between experiments and user code (e.g., high fidelity simulations and models). Linking the experimental capabilities of LES with the turbulence-simulation capabilities of DNS leads to geometric and realistic conditions. LES is an effective tool today in lab-scale devices. The capabilities of LES could be improved with additional R&D and, in the future, provide a high-fidelity simulation tool for the commercial sector. In experiments, data that is highly resolved spatially is needed with whatever method used to solve it, rather than input-outputs. LES provides this capability.

- Development of key validation experiments is part of the layering process. The layered numerical tools will be coupled with a well-defined suite of validation experiments to focus on individual topics important to end-users.

- LES development is currently focused on lab-scale, application-relevant conditions. As a result, a simulation validated with experiments is provided for an application. This can be used to improve DNS for a given condition. DNS helps users focus on smaller scales, which facilitates development of requirements to feed back into a LES sub-model and further reduce to RNS. The benefit is that there is a focal point with common geometry and set of operating conditions to reference. DNS will assist with model development, validation, and scientific discovery.

- To assure that research efforts are relevant to end-users, developers of DNS, LES, and RANS methodologies should work together, with focus on end-user goals. A reasonable approach might be the development of detailed experiments focusing on a small number of industrial priorities.

CFD R&D Priority: <u>Develop an Experimental Test Facility to Produce Consistent Validation Datasets</u>

- There are different levels of validation: fundamental and experimental. Validation capability is needed to reliably predict heat-flow and heat-transfer fundamentals.

- Industry has an end goal of what they want the model to predict and against what sorts of problems they would like to test their codes. When designing experiments for a facility, the problem must be relevant to the tools used by industry because they pose different requirements on the experiment. Part of the challenge is identifying industry's need.
- One approach is to start with experiments that have relatively simple codes, get this correct, and then move to tougher problems. This approach can help identify the best place for experiments (e.g., the Combustion Laboratory or BERL).

Appendix D. CFD Benefit Analysis Calculations

Energy Savings

The industrial energy savings from significant improvements in CFD modeling for burners and the resulting burner design improvements were estimated to be 55 Tbtu/year in 2010 and 973 Tbtu/year in 2020. This is based on energy use data from Energy Information Administration's (EIA) 1998 Manufacturing Energy Consumption Survey (MECS) and a conservative growth rate of 1% per year for burners, boiler, and process heaters.

> **Benefits and Impacts of Quantitative CFD Design Methods**
>
> - **Improved Energy Efficiency**—heat is transferred to the load more efficiently, thereby reducing fuel use
> - **Facilitates Alternative Energy Use**—combustion system impacts from alternative fuels can be evaluated, thereby contributing to energy security

Future energy use is estimated for two scenarios: "Scenario 1" – where no significant burner improvements occur, and "Scenario 2" – where CFD improvements lead to significant efficiency improvement. The assumed market penetration is the percentage of boilers, furnaces and process heaters that have improved efficiency due to the CFD advancements. The efficiency improvement is the percentage of energy that is *not* used by the boiler/process heaters that are improved through CFD. The total % energy savings are calculated by multiplying the market penetration by the efficiency improvement. The data results are as follows:

Industrial Energy Use

	Current Energy Use 1998 MECS* TBtu/Year	Energy Use in 2010 SCENARIO 1 TBtu/Year	Energy Use in 2010 SCENARIO 2 TBtu/Year	Energy Use in 2020 SCENARIO 1 TBtu/Year	Energy Use in 2020 SCENARIO 2 TBtu/Year
Boilers	6,020	6,783	6,756	7,493	7,013
Furnaces & Process Heaters	6,194	6,980	6,952	7,710	7,217
Total Industrial Burner Energy Use	12,214	13,763	13,708	15,203	14,230
Total Fuel Energy Use	17,741	20,053	19,998	22,083	21,110
Total Energy Savings			**55**		**973**

Scenario 1 = CFD modeling for burner design continuing to develop gradually, assumes 1% market growth
(No significant energy efficiency improvement in burners)
Scenario 2 = Significant Improvement in CFD modeling for burner design, assumes 1% market growth
2010 Effects of CFD Improvement = 2% efficiency improvement and 20% market penetration
2020 Effects of CFD Improvement = 8% efficiency improvement and 80% market penetration

* 1998 Manufacturing Energy Consumption Survey Published by the Energy Information Administration

The cost savings benefit from reduced fuel consumption is calculated by multiplying the savings above (55 and 973 Tbtu / year) and the fuel cost projections based on government estimates ($/Million Btu). The cost savings from reduced fuel use with Scenario 2, which assumes significant improvement in CFD modeling, are $159,000 for 2010 and $2.8 Million for 2020. The calculations are as follows:

Total Fuel Savings

		2010	2010	2020	2020
	$/Million BTU*	TBtu/Year	$/Year	TBtu/Year	$/Year
Total		**55**	**$ 158,730**	**973**	**$ 2,808,078**
Natural Gas	3.21	33.00	$ 105,930	583.80	$ 1,873,998
Coal	1.36	16.50	$ 22,440	291.90	$ 396,984
Oil	5.52	5.50	$ 30,360	97.30	$ 537,096

* $/Million BTU estimates are from 2002 GPRA analysis (unpublished)

Emissions Reductions

The industrial emissions reductions from significant improvements in CFD modeling for burners and the resulting burner design improvements were estimated to be $1.0 Billion for 2010 and $5.4 Billion for 2020. The emission rates are based on the 1994 EIA/MECS Industrial Average Carbon Intensity Rate (million carbon equivalent units per quadrillion BTU) and emission rates based on a fuel mix of 60% natural gas, 30% coal, & 10% oil (metric tons per billion KWH for NOx and SO_2).

Benefits and Impacts of Quantitative CFD Design Methods

- **Reduced NO_x, SO_x, CO, and Particulate Emissions**— emissions characteristics can be predicted to achieve desired emissions profiles, thereby reducing pollution and the costs associated with regulatory compliance and non-compliance

As in the energy use calculations, the growth in energy use was estimated to be 1% per year, a conservative estimate for burner, boiler, and process heater and the emissions are calculated for two scenarios: “Scenario 1” – where no significant burner improvements occur, and “Scenario 2” – where CFD advances lead to significant emission reductions. In “Scenario 2”, the increased market penetration and efficiency improvements lead to additional emission reductions (2% for 2010 and 5% for 2020). The data results are as follows:

Industrial Emissions	Current Emissions 1998 MECS Million Metric Tons/ Year	Emissions in 2010 SCENARIO 1 Million Metric Tons/ Year	Emissions in 2010 SCENARIO 2 Million Metric Tons/ Year	Emissions in 2020 SCENARIO 1 Million Metric Tons/ Year	Emissions in 2020 SCENARIO 2 Million Metric Tons/ Year
Boilers					
NOx 1	2.82	3.18	3.10	3.51	3.12
SO2 2	3.88	4.37	4.27	4.83	4.30
Carbon Units 3	103.30	116.40	113.61	128.58	114.33
Furnaces & Process Heaters					
NOx 1	2.90	3.27	3.20	3.62	3.22
SO2 2	3.99	4.50	4.39	4.97	4.42
Carbon Units 3	106.29	119.78	116.91	132.30	117.64
Total Emissions					
NOx	5.73	6.45	6.30	7.13	6.34
SO2	7.88	8.87	8.66	9.80	8.72
Carbon Units	209.59	236.17	230.52	260.88	231.98
Total Emission Reduction			**2010**		**2020**
NOx			**0.15**		**0.79**
SO2			**0.21**		**1.09**
Carbon Units			**5.65**		**28.91**

Scenario 1 = CFD modeling for burner design continuing to develop gradually, assumes 1% market growth
Scenario 2 = Signficant Improvement in CFD modeling for burner design, see above for energy details
+ an additional 2% emission reduction for 2010 and 5% reduction for 2020

1 - Calculated using the estimate of NOx emissions per KWH of electricity (1600 metric tons/billion KWH)
(This rate uses a fuel mix of approximately 60% natural gas, 30% coal, and 10% oil)
2 - Calculated using the estimate of SO2 emissions per KWH of electricity (2200 metric tons/billion KWH)
(This rate uses a fuel mix of approximately 60% natural gas, 30% coal, and 10% oil)
3 - Calculated using the 1994 EIA/MECS Industrial Average carbon intensity rate 17.16 mmtc/quadrillion BTU
MECS data is from the Manufacturing Energy Consumption Survey by the Energy Information Administration

Emissions Reductions (cont'd)

The cost savings benefit from the emission reductions is calculated by multiplying the savings per year above (for example in 2010: 0.15 NOx, 0.21 SO_2, & 5.65 Carbon Units Million metric tons/year) and the emission control/treatment costs ($/Metric ton) from EIA estimates. The estimated savings are $1.0 Billion for 2010 and $5.4 Billion for 2020.

Total Emission Control Savings		**2010**	**2010**	**2020**	**2020**
	$ / Metric Ton	Metric Ton/Yr	$/Year	Metric Ton/Yr	$/Year
Total			**$ 1,051,614,563**		**$ 5,380,855,906**
NOx	$ 1,619	154,387	$ 249,952,184	789,960	$ 1,278,944,521
SO2	$ 237	212,282	$ 50,310,789	1,086,194	$ 257,428,070
Carbon Units	$ 133	5,649,260	$ 751,351,590	28,905,890	$ 3,844,483,315

$/Metric Ton for CO2 is from EIA, "Analysis of Strategies for Reducing Multiple Emissions from Power Plants: SO2, NOx, and CO2"
$/Metric Ton for NOx and SO2 is from the EIA, "The Effects of Title IV of the CAA Amendments of 1990 on Electric Utilities"

Development Cost Savings

Development costs for burners, boilers, furnaces, and process heaters include the direct costs associated with engineering, equipment design, and equipment evaluation, as well as maintaining sufficient R&D resources to evaluate new technologies for product development. The development cost savings from significant improvements in CFD modeling for burners and the resulting burner design improvements were calculated to be $ 7.1 Million/year in 2010 and $15.6 Million in 2020. These savings are based on an estimate of 30,000 boilers and 60,000 furnaces in 1998 with an assumed market growth rate of 1%. The development cost for each unit assumes of 20 burners per unit at $5000 per burner, with 15% of the cost of each burner due to development. Development cost savings are estimated to be 10% in 2010 and 40% in 2020. The data results are as follows:

Benefits and Impacts of Quantitative CFD Design Methods

- **Improved Product Quality**—byproducts that contact the load can be reduced and temperature can be more reliably controlled, thereby producing more consistent products
- **Reduced Development Costs**—relying on simulations to evaluate design options reduces fabrication and testing time and costs, and reduces the reliance on trial and error
- **Better Burner Designs**—optimally designed burners that are integrated into the entire combustion system are more responsive to application requirements

Total Development Cost Savings

		2010	2010	2020	2020
	Development Cost per unit	# Units Sold	Savings $/Year	# Units Sold	Savings $/Year
Total			**$ 3,533,298**		**$ 15,599,844**
Boilers	$ 33,333	390	$ 1,299,987	431	$ 5,746,609
Furnaces	$ 33,333	670	$ 2,233,311	739	$ 9,853,235

Development savings = 20 burners per unit * $5000 per burner * (1/3 cost per burner for R&D * % savings)
Assumes CFD development cost savings are 10% in 2010 and 40% in 2020.
Number of units sold per year includes retrofits.

Customer Service Cost Savings

> **Benefits and Impacts of Quantitative CFD Design Methods**
>
> - **Faster Problem Diagnosis with Expanded Response Options—** more rapid and robust solutions to customer problems improves performance and reduces manpower requirements and downtime

Customer service costs for burners, boilers, furnaces, and process heaters include the direct costs associated with engineering assistance, problem diagnosis, and equipment evaluation, as well as maintaining sufficient R&D resources to assist with problem diagnosis when needed. Improved CFD tools could lead to reductions in costs from faster problem equipment/process evaluation, and reduced demand for technical resources. The customer service cost savings from significant improvements in CFD modeling for burners and the resulting burner design improvements were estimated to be $26.8 Million/year in 2010 and $59.1 Million/year in 2020. These savings are based on an estimate of 30,000 boilers and 60,000 furnaces in 1998 with an assumed market growth rate of 1%. The customer service/technical assistance cost for each unit assumes 25% of all units will require service per year at a cost of $5000 per service. Customer service cost savings are estimated to be 10% in 2010 and 40% in 2020. The results are summarized below:

Total Customer Service Cost Savings

	Savings per problem	2010 Total # of Units	2010 Savings $/year	2020 Total # of Units	2020 Savings $/year
Total Savings			**$ 13,381,000**		**$ 59,124,000**
Boiler & Furnace Units -2010	$ 500	107048	$ 13,381,000		
Boiler & Furnace Units -2020	$ 2,000			118248	$ 59,124,000

Assumes 25% of units require technical assistance.
Assumes technical assistance costs $5000 for each problem.
Assumes CFD will reduce costs 10% in 2010 and 40% in 2020.

Total Industry Cost Savings

The overall cost savings from significant improvements in CFD modeling for burners and the resulting burner design improvements were calculated to be $ 1.1 Billion/year in 2010 and $5.5 Billion in 2020. These savings are calculated from totaling the savings from all categories:

Industrial Cost Savings

	2010	2020
Total Industry Savings	**$ 1,068,687,591**	**$ 5,458,387,828**